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The propagation of nonlinear waves induced by a shock impulse in a linear atomic chain of finite but large length is investigated numerically with a model interatomic potential. The shock impulse is initiated by giving the first atom in the chain an initial velocity υ_i toward its neighbor. We find that there exists a velocity υ_c such that for $\upsilon_i > \upsilon_c$ a soliton is produced by this impulse with a constant energy and supersonic velocity υ_s. Studies of the motion of the atom during the passage of this soliton reveal a behavior similar to that expected from the collision of hard spheres. However, for $\upsilon_i < \upsilon_c$ the induced pulse propagates below the speed of sound and gradually disperses through the emission of phonons. In the supersonic regime, $\upsilon_i > \upsilon_c$, we find that there exists a velocity υ_m such that if $\upsilon_i > \upsilon_m$, then $\upsilon_s < \upsilon_i$, but if $\upsilon_i < \upsilon_m$, then $\upsilon_s > \upsilon_i$. Finally, in agreement with earlier studies using other model potentials, we find that if υ_i is large enough, a soliton can be generated with sufficient energy to spall an atom from the end of the chain.

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Dynamics of Solitary Waves Induced by Shock Impulses in a Linear Atomic Chain*

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Abstract

The propagation of nonlinear waves induced by a shock impulse in a linear atomic chain of finite but large length is investigated numerically with a model interatomic potential. The shock impulse is initiated by giving the first atom in the chain an initial velocity v_i toward its neighbor. We find that there exists a velocity v_c such that for $v_i > v_c$ a soliton is produced by this impulse with a constant energy and supersonic velocity v_s. Studies of the motion of the atom during the passage of this soliton reveal a behavior similar to that expected from the collision of hard spheres. However, for $v_i < v_c$ the induced pulse propagates below the speed of sound and gradually disperses through the emission of phonons. In the supersonic regime, $v_i > v_c$, we find that there exists a velocity v_m such that if $v_i > v_m$, then $v_s < v_i$, but if $v_i < v_m$, then $v_s > v_i$. Finally, in agreement with earlier studies ~~on~~ other model potentials, we find that if v_i is large enough, a soliton can be generated with sufficient energy to spall an atom from the end of the chain.

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Introduction

Since J. Scott Russell's observation (1834) of solitary waves on the surface of water, many other physical systems have been found to support the propagation of solitons. Initial analytic studies by Korteweg and de Vries [1] has resulted in an equation (KdV) which became a model for nonlinear wave propagation in fluid dynamics, plasma physics, optical communications, and other discrete nonlinear lattices. Zabusky and Kruska [2] found a particular solution to the KdV equation in the form of stable pulses that can retain their initial shapes even after colliding into one another. These pulses were termed solitons as they behave like stable particles.

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Due to their remarkable properties, solitons have been proposed as a mechanism for energy transport in biological systems as well as in solids. Certain types of nonlinear discrete lattices such as the Toda model [3] are found to be integrable and have exact soltonic solutions. A few nonlinear models for interatomic potentials to some degree of approximation can be reduced to the KdV equation and hence admit solitons.

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Studies of shock compression in solids and in energetic materials have been undertaken normally within the framework of continuum mechanics where macroscopic properties such as the temperature, pressure, and velocity profiles of atoms

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near the shock front are obtained. The continuum approach, however, does not include the dispersion in a discrete anharmonic lattice that may lead to an unsteady shock front, a result which is not allowed in hydrodynamic equations. Discrete models for shock wave propagation can provide physical details of the shock front and of individual atoms on a microscopic scale. Discrete models can also be used to study chemically sustained shock waves [4,5]. A large quantity of theoretical and experimental works on shock compression has been published, e.g., Ref. [8]. Some previous works have suggested that solitonic behavior [6,7] of a steady shock can result in the breaking of chemical bonds [8]. Moreover, the solitons initiated without shock waves in the Toda chain were shown numerically to cause fragmentation [9]. In this work, we study the propagation of solitons generated by varying the impact velocity of an instantaneous shock upon a linear chain. Other aspects associated with shock compression such as thermal excitation and chemical reaction in a heterogeneous lattice will be left to further studies.

In addition to existing models for interatomic potentials of Lennard-Jones, Morse, and Rydberg types, we can construct a simple potential that describes a repulsive interaction at short distance, attractive interaction within a finite range and vanishing at infinite, written as

$$V_{i,j} = C[1 - K(x_i - x_j)]e^{-K(x_i - x_j)} \tag{1}$$

where x_i is the position of the ith atom and K and C are positive constants proportional to the equilibrium separation and binding energy, respectively. The order of i and j is chosen such that $x_i > x_j$. If we consider only nearest neighbor interactions, Hamilton's equation for a one-dimensional lattice with free ends can be reduced to

$$\frac{d^2Y_i}{dT^2} = (Y_{i+1} - Y_i - 2)e^{-(Y_{i+1}-Y_i)} - (Y_i - Y_{i-1} - 2)e^{-(Y_i - Y_{i-1})} \tag{2}$$

where Y and T, respectively, are the atomic position and time in dimensionless units. In the next section, we show a solution of the above system of ordinary differential equations obtained by using numerical algorithms. Analytical solutions in the continuum limit will also be presented.

Results

The dimensions used in this calculation were scaled such that each unit of velocity, distance, and time correspond to 14.29 km/s, 1.6 Å, and 1.21×10^{-14} s, respectively. These values were based on an atomic mass of 14 amu, lattice spacing of 3.2 Å, and binding energy of 4 eV. The number of atoms in the chain is between 150 and 500.

The shock impulse is initiated by giving the first atom in the chain an initial velocity v_i, termed the impact velocity, toward its neighbors. The shock propagates further into the chain through interaction between neighboring atoms. At any moment, the position of the shock front can be defined as that of the last atom with the highest velocity, adjacent to the remaining atoms which are not yet disturbed.

Each atom is displaced in the same direction as the shock front passes. This translation is similar to the result of a collision of hard spheres. The graph of atomic velocity versus chain length shows a sharp pulse at the shock front [Fig. 1(a)]. Below a limit value v_c of the impact velocity, the amplitude of the pulse decreases (or disperses) as the front advances further into the lattice. This dispersion vanishes when the speed of the front reaches a value v_s which requires an impact velocity v_c. Analytical calculation (given below) in the long wavelength limit shows that v_s is the speed of sound in the lattice and also that it is a minimum velocity a soliton must have.

For $v_i > v_c$, the amplitude of the pulse remains constant in time as it passes through the lattice. Furthermore, the pulse travels with a constant speed and energy until its gets reflected at the end of the chain. These results suggest solitonic behavior for the shock pulse (atomic velocity). The plot of this pulse in time [Fig. 1(b)] is similar to a hyperbolic secant function which is indeed a result obtained analytically in continuum limit. Supersonic solitons that emerge from a collision initiated by impacts upon both ends of the chain retain their initial shapes (Fig. 2). Also in this supersonic regime, there exists a value $v_m > v_c$ such that the speed of soliton (or shock front) is found to be faster than the impact velocity if $v_i < v_m$, and slower if $v_i > v_m$. This characteristic is illustrated in Figure 3.

Depending on the value of the impact velocity, the energy of the soliton can attain a critical value to spall an atom from the end bond, which is the most weakly bound atom in the chain. This amount of energy is independent of the total number of atoms in the chain. Therefore, it is possible to have a stream of shock impulses acting on a lattice to generate a sequence of solitons with sufficient energy to break

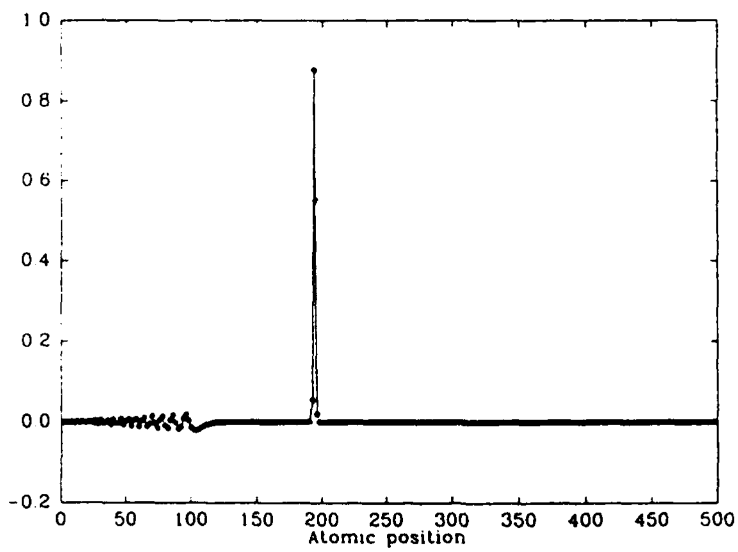

Figure 1(a). Atomic velocities vs. atomic positions. $v_i = 1.4$, $N = 250$ atoms.

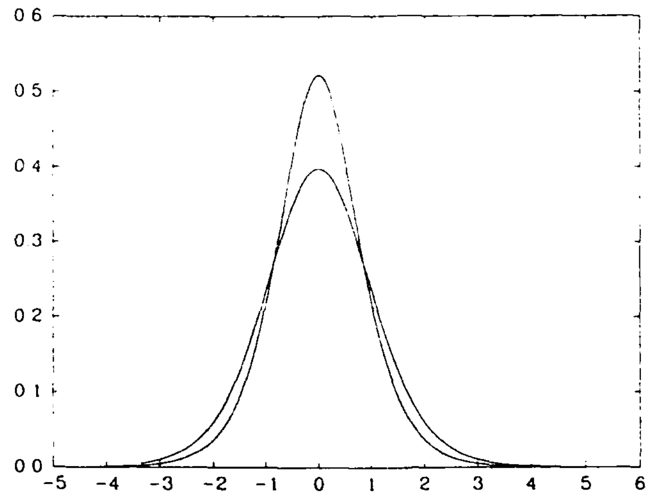

Figure 1(b). Atomic velocity vs. time. The curve with lower peak is obtained by numerical method for a discrete lattice. The one with higher peak is an analytic solution, Eq. (6) in continuum limit, $v_i = 0.6$, $N = 250$ atoms.

away the atoms one by one from a free end [9]. This may suggest an intrinsic mechanism for the breaking of chemical bonds without detonation by shock waves.

We now show an approximate analytic solution. In the long wavelength limit, the continuous version of Eq. (2) can be obtained by using

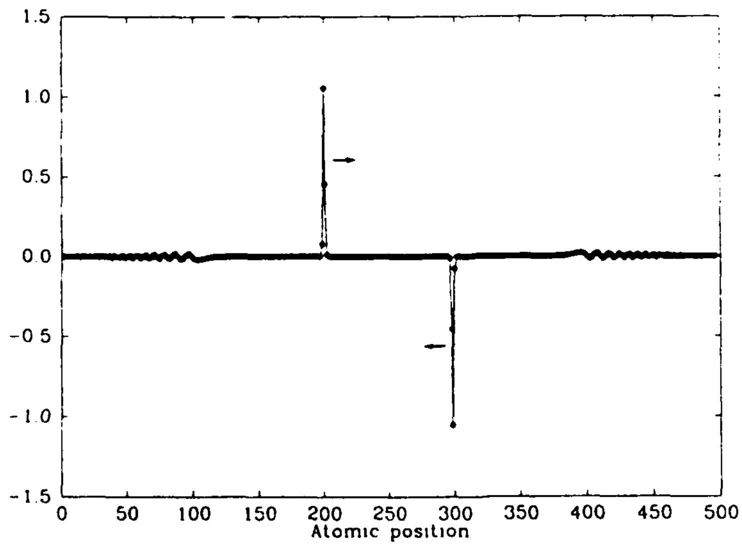

Figure 2(a). Collision of two solitons initiated by the same impact velocity on both ends of the chain. $v_i = 1.5$, $N = 250$ atoms.

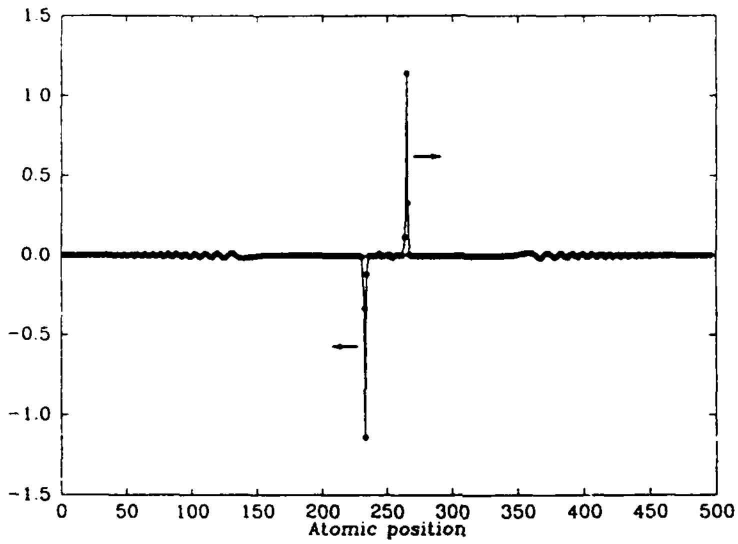

Figure 2(b). Two solitons emerge intact after the collision.

$$R_{i\pm1} = R_i \pm \frac{dR_i}{di} + \frac{1}{2}\frac{d^2R_i}{di^2} \pm \frac{1}{3!}\frac{d^3R_i}{di^3} + \frac{1}{4!}\frac{d^4R_i}{di^4} \pm \cdots \tag{3}$$

with the atomic displacement R_i being used instead of Y_i. First, Eq. (2) is expanded about the atomic equilibrium position up to second-order terms to obtain an ap-

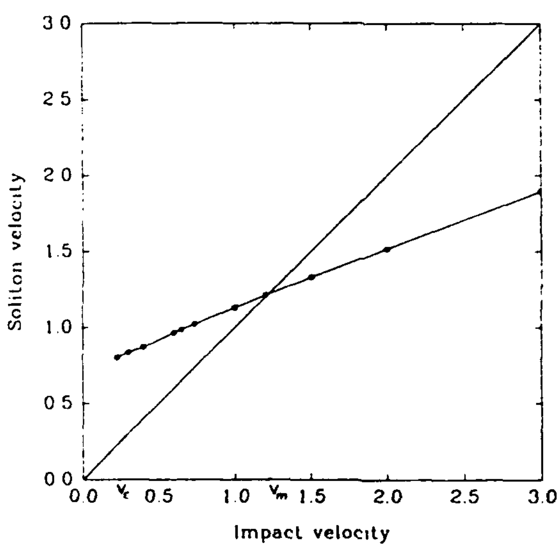

Figure 3. Soliton (or shock front) velocity vs. impact velocity. The supersonic soliton is generated only in the region $v_l > v_c$.

proximate discrete equation. The resulting equation is then transformed into the continuum limit using Eq. (3) and keeping only leading terms up to fourth order in derivatives to obtain

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$$e^2 \frac{d^2R}{dT^2} = \frac{d^2R}{di^2} - 2\frac{d^2R}{di^2}\frac{dR}{di} + \frac{1}{12}\frac{d^4R}{di^4}; \tag{4}$$

Let $z = K(x - vt)$ be a coordinate moving with the wave; then Eq. (4) becomes

$$\frac{\partial S}{\partial \tau} + \frac{1}{2} S \frac{\partial S}{\partial z} + \frac{1}{24}\frac{\partial^3 S}{\partial z^3} = 0 \tag{5}$$

where $S = \partial R/\partial T$ being the atomic velocity, $\omega = T/t$, $\tau = 32\alpha^{-1}T$, and $\alpha = (eKv/\omega)^2 - 4$. This is the Korteweg–de Vries equation, which can be shown to admit a particular solution in the form

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$$S = S_\infty + \frac{\sigma}{4}\operatorname{sech}^2\left(\frac{\sqrt{\sigma}}{2} z\right) \tag{6}$$

with $\sigma = \frac{3}{4}\alpha(Kv/\omega)$. The stability of this solution requires α to be positive or

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$(2/e)\sqrt{C/m}$ with m being the atomic mass. This minimum is equal to the speed of sound traveling in the lattice, obtained analytically by solving Eq. (2) in the long wavelength limit. The soliton therefore exists only in a supersonic regime. Figure 1(b) shows a comparison between a continuous solution (6) and a discrete solution (numerical).

Discussion

It has been known that nonlinear lattices are not integrable except in very few models (e.g., the Toda exponential potential). Nonlinear interactions have a wide range of applications in many physical systems. Moreover, the balance between the nonlinear interaction in the lattice and the dispersion in the medium may give rise to interesting properties such as the recurrence phenomenon [10] (Fermi–Pasta–Ulam) and nondispersive solitary waves. Most other work [6–8] on shock waves and solitons in solids considered only the case of steady shocks. Although Karo has observed single soliton generated by impacting one end of the chain [11], the dynamical behavior of the lattice in response to shocks with different impact velocities has not been investigated in detail. By considering the shock impulse, we found that the shock front (or soliton) can propagate only with a supersonic speed, and that it is not always linearly proportional to the impact velocity. The energy delivered to a crystalline lattice by shock waves, as shown in this simplified model, is transported by lattice solitons. Chemical bonds within the lattice may break when the energy carried by the shock-induced solitons attain a certain critical threshold. Not only the bonds near the end of the lattice are broken up, but also those far away from the end as we have observed in the case of a sequence of impulses or a steady shock [12].

We also found a minimum value of the impact velocity for the shock to generate a soliton that exists only in a supersonic regime. The speed of the soliton varies with the impact velocity but is time-invariant and independent of the length of the chain. The shock front (determined by the position of soliton) will continue to travel with the same speed when it first impacts upon the lattice only if the impact velocity has a particular value v_m. If the impact velocity falls below v_m, the front propagates faster and otherwise if above that value. The different behavior of the shock front when the impact velocity is below and above v_m arises most likely from the nonlinearity, an intrinsic property of the lattice. For an impact velocity greater than v_m, the force exerted by a shock is able to suppress the nonlinearity and therefore results in a slower speed of the shock front. Furthermore, it has been known that nonlinearity enhances the energy transport in a disordered lattice [13].

Our finding suggests a mechanism of energy transport in a lattice by a shock impulse, and determines how fast a shock front can propagate in a material given the impact velocity. Other aspects of shock compression in a lattice are subject to future works.

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